Adjoint methods for 3D remote sensing

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NASA Goddard Institute for Space Studies

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Outline:

Adjoint methods for 3D remote sensing

- ***Why do we need 3D radiative transfer?***
- ***Why do we need adjoint methods?***
- ***What is an adjoint method?***

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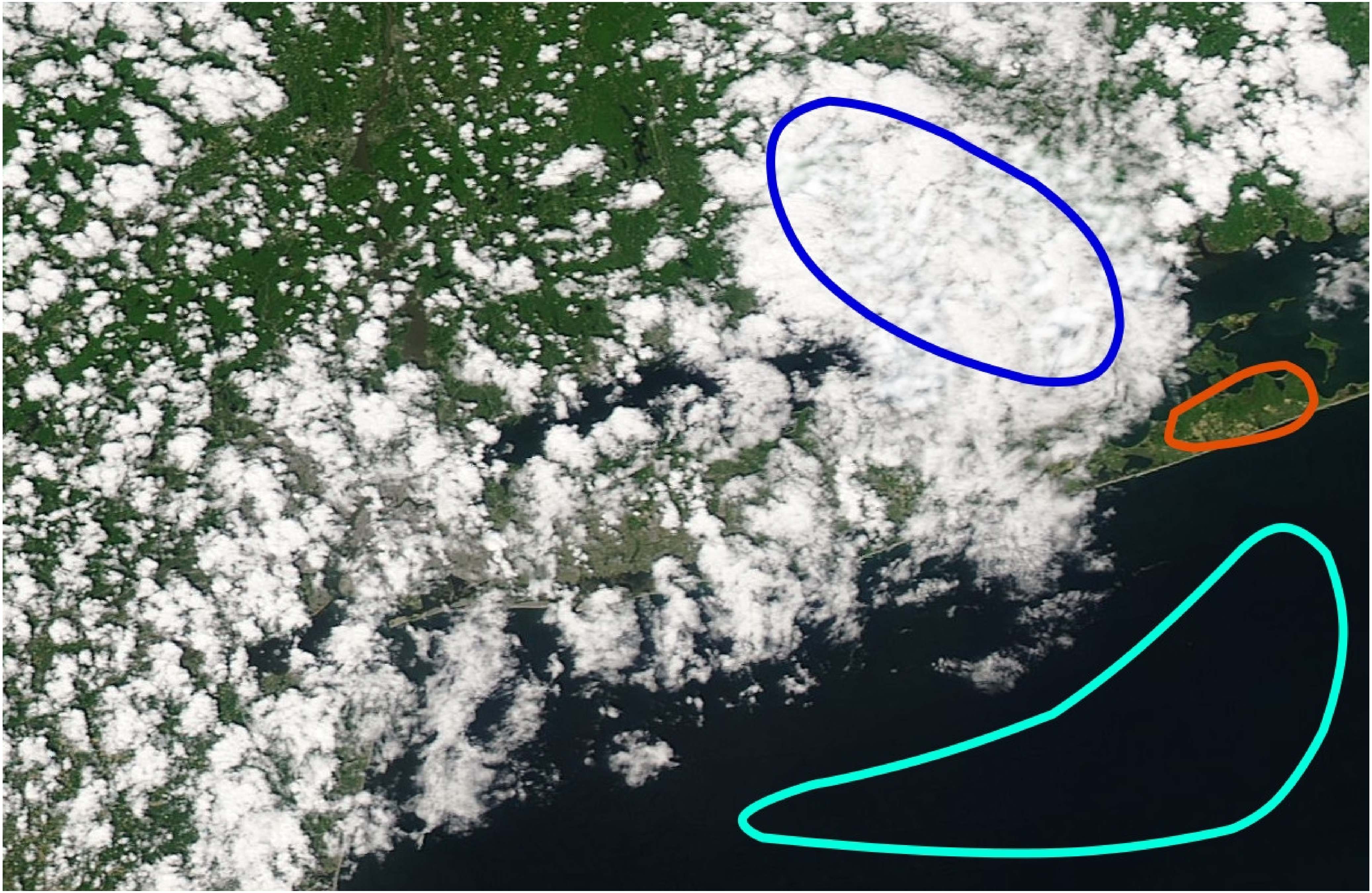
Retrievals in 1D can work well



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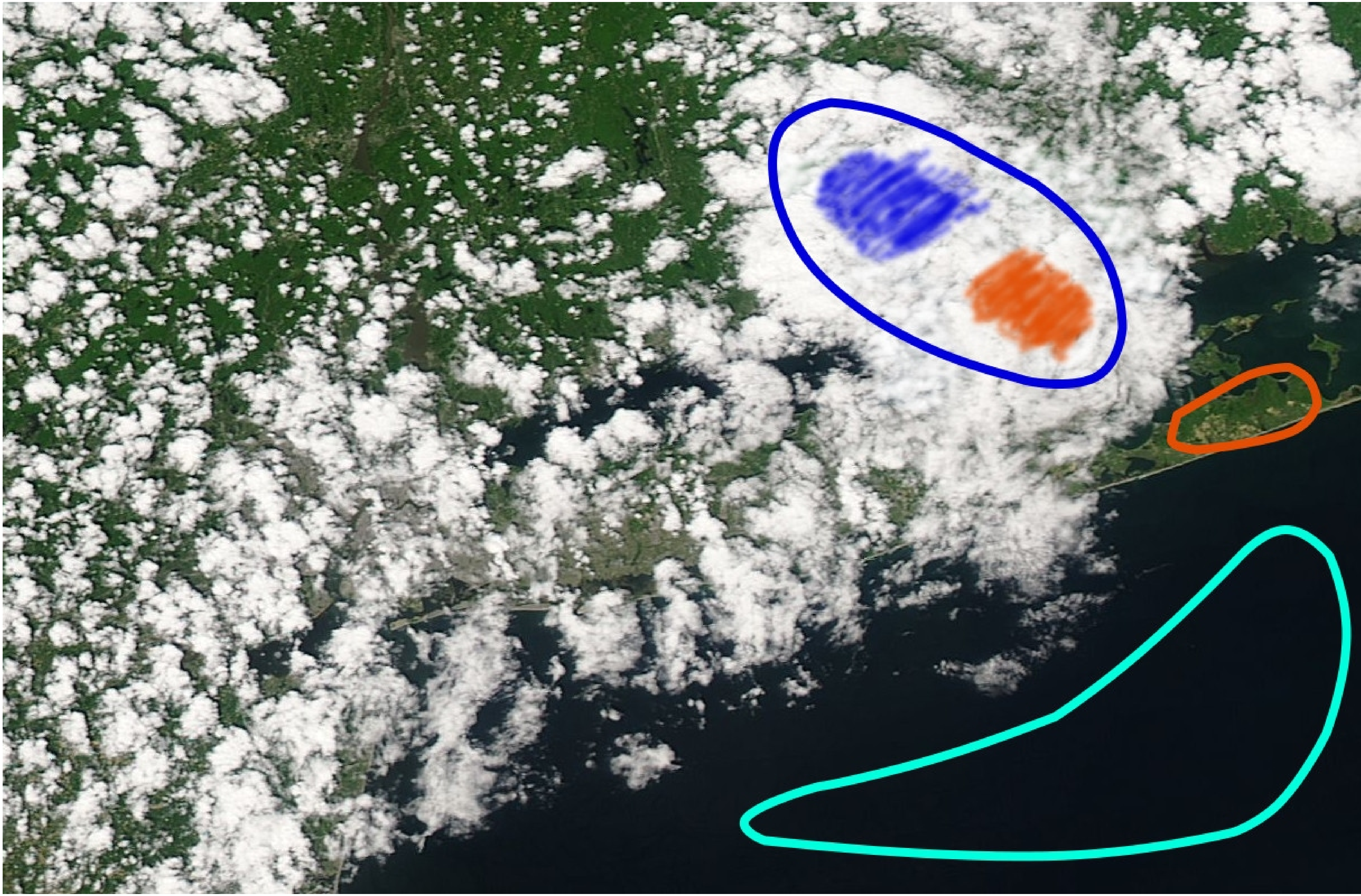
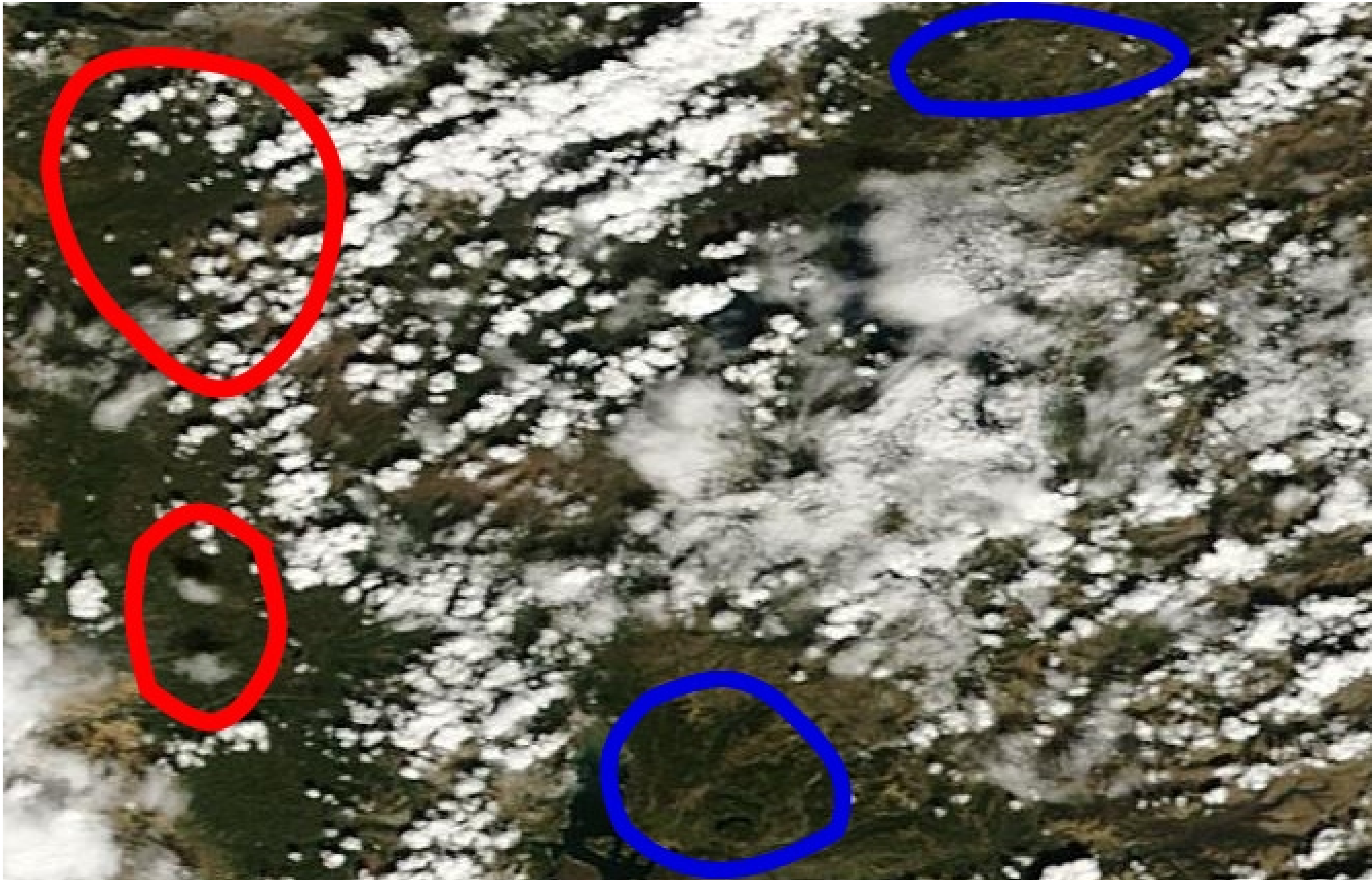
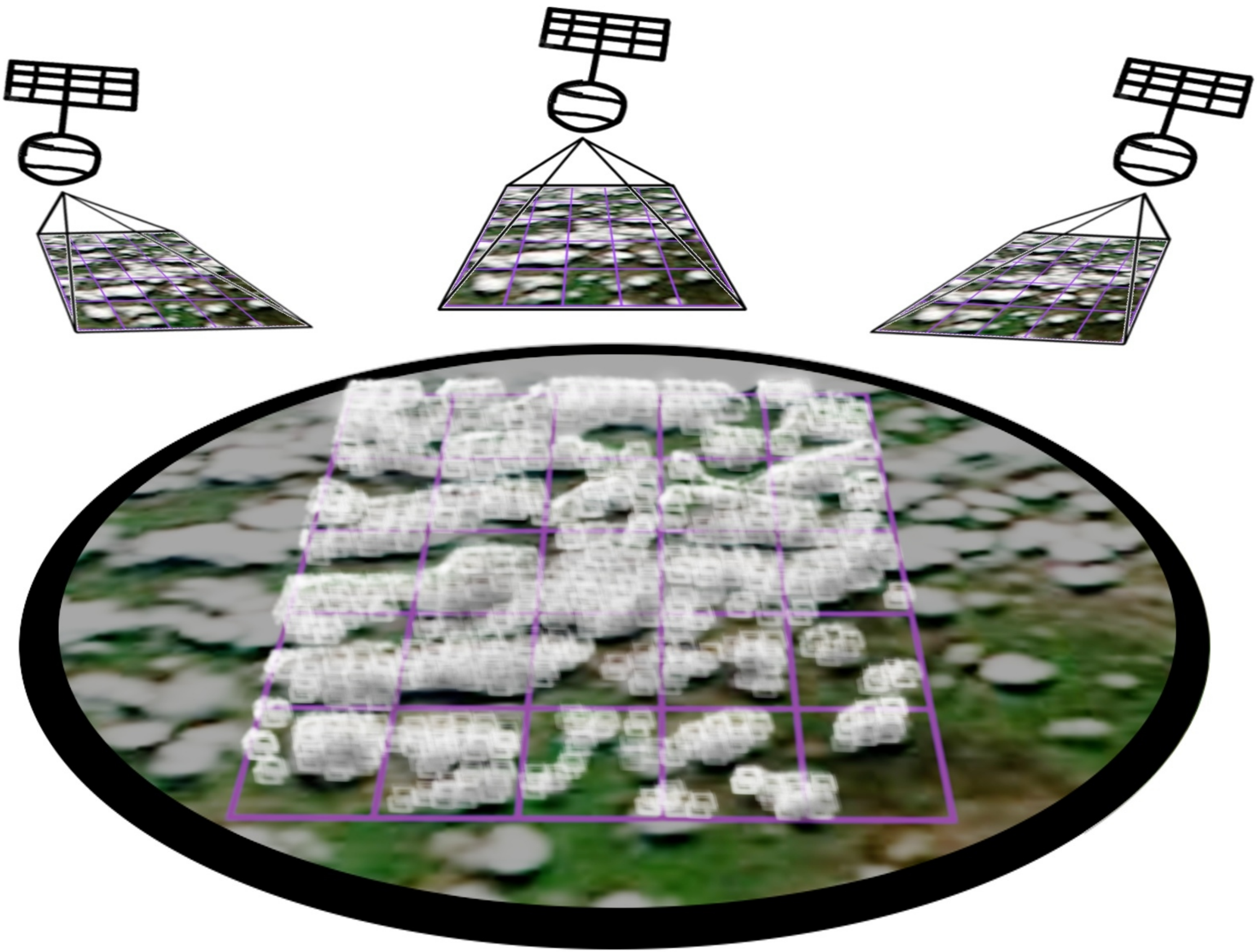


Retrievals in 3D can extend coverage

Retrievals in 3D can exploit 3D effects



The cost:
dependent pixels and 3D radiative transfer



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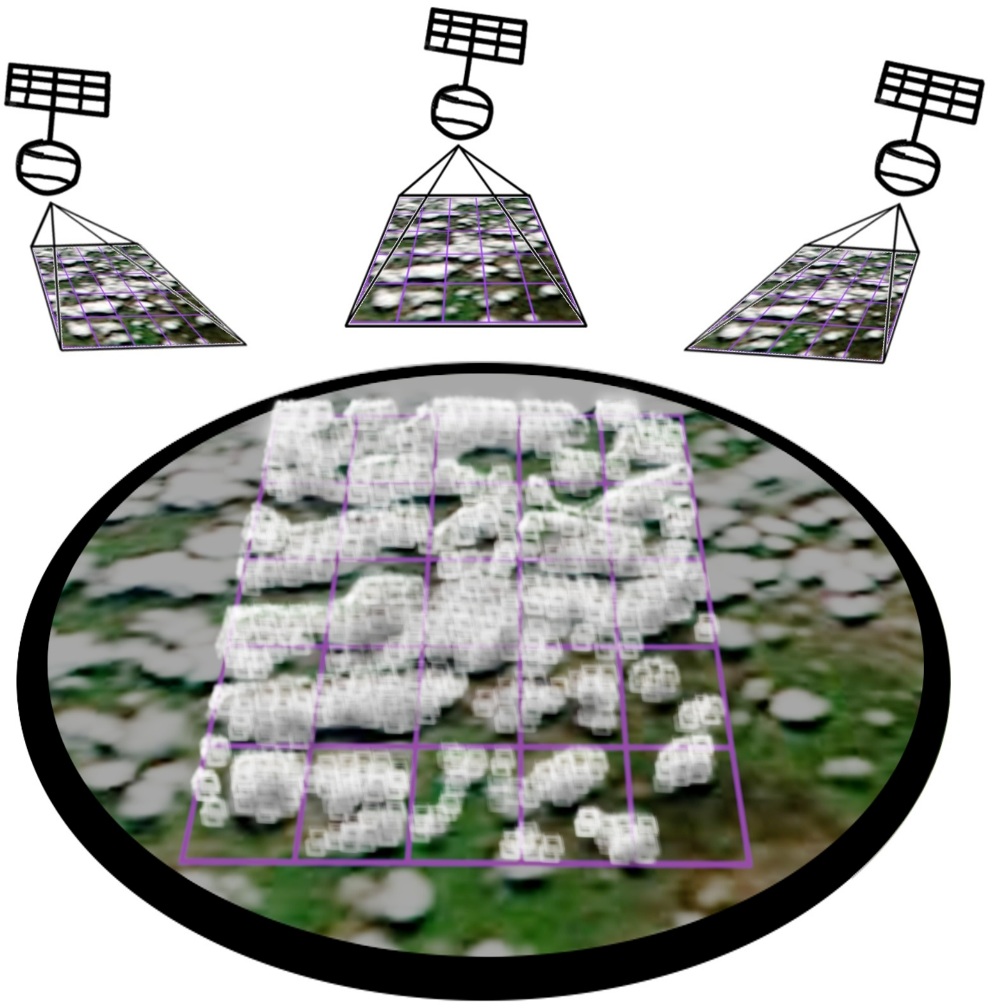
Cloud representation:

Three-dimensional cloud



Consider 3D retrievals to extend coverage to broken cloud fields

Solver 3D VRTE

- SHDOM [Evans,1998 and 2014]
- Polarization [Doicu, Ef., Tr. 2013]
- Adjoint derivative [Martin, 2014]

Inverse problem

- Retrieval of 1D cloud properties [Evans, 2008]
- Stability and data requirements?

Cloud representation:

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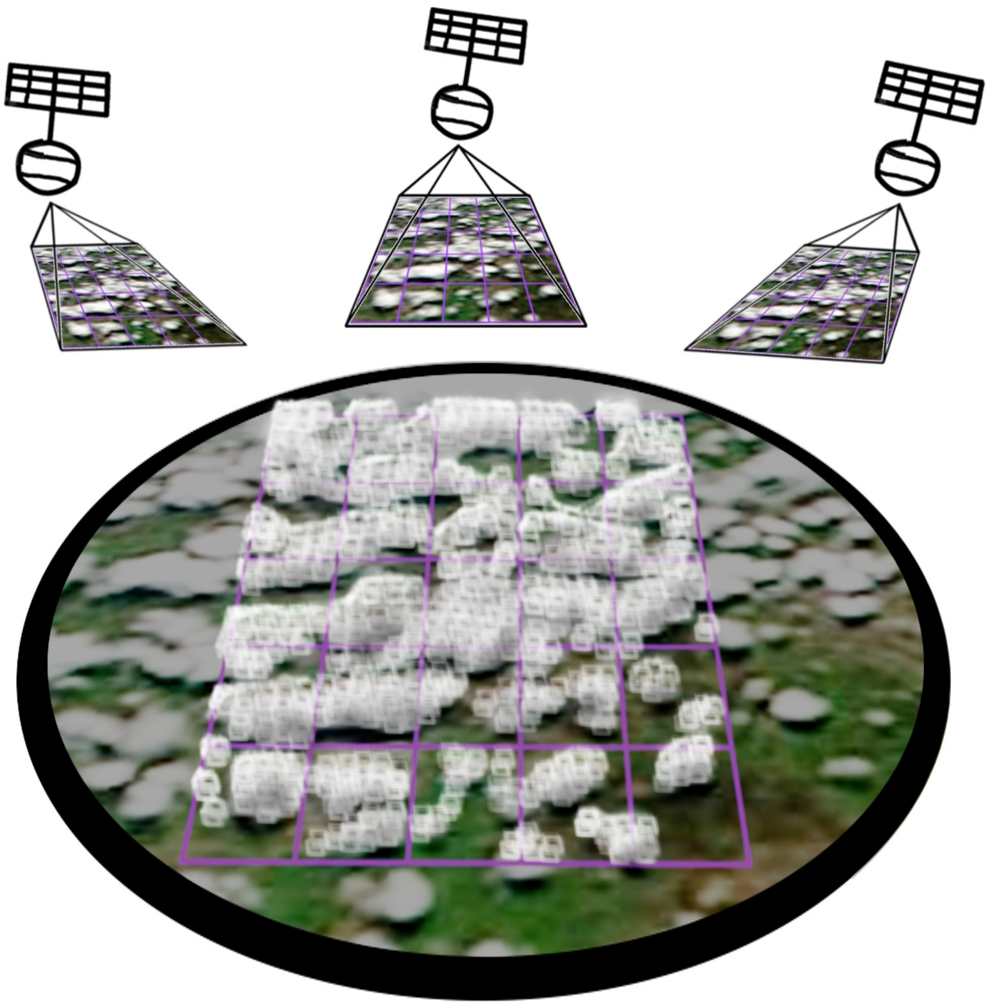

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Inverse problem

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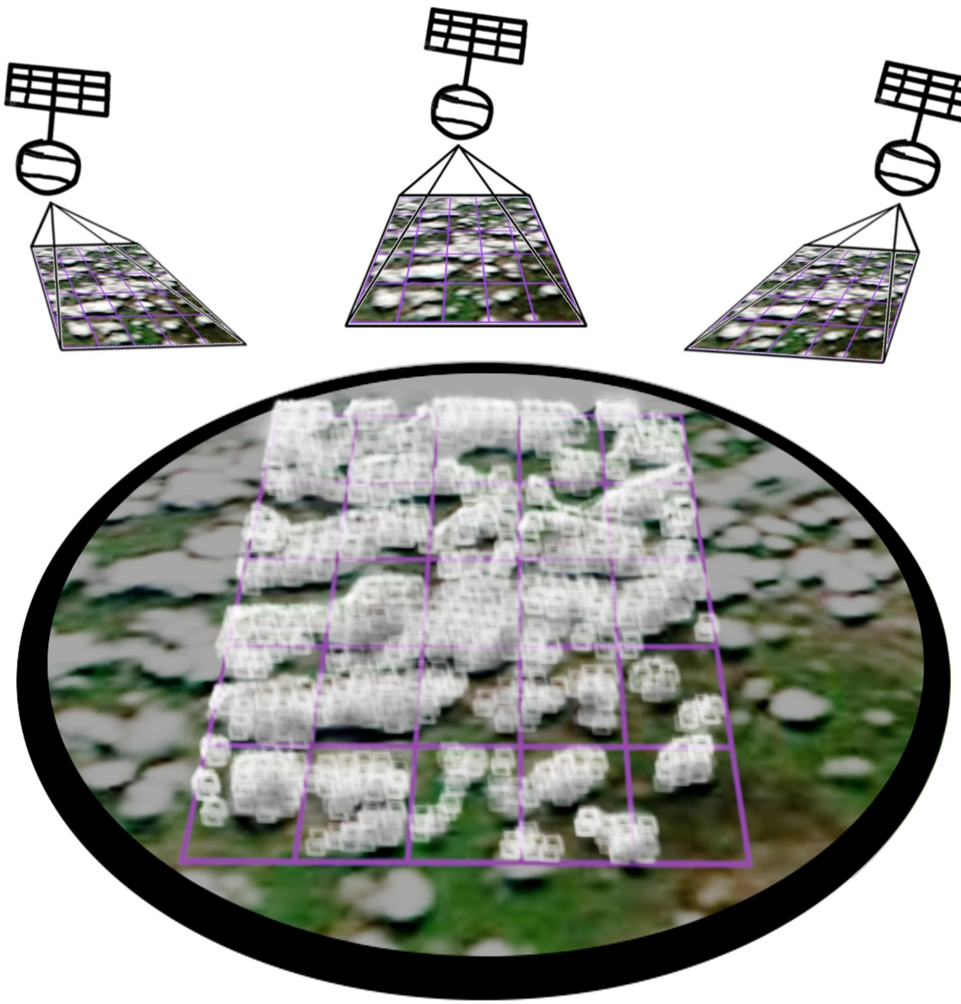
- Stability and data requirements?

How do we represent clouds for doing 3D retrievals of the atmosphere and surface?

Cloud representation:

Three-dimensional cloud



Measurements (future)

- Passive polarimetric imaging and active LIDAR and RADAR.

  ~100 images

  x

  ~10,000 pixels per image

  =

  ~1,000,000 total measurement constraints

Unknown parameters to retrieve

- *Cloud, aerosols and surface for each patch*

  ~1,000 volume and surface elements

  X

  ~10 properties (aerosol, cloud or surface)

  =

  ~10,000 total unknown parameters

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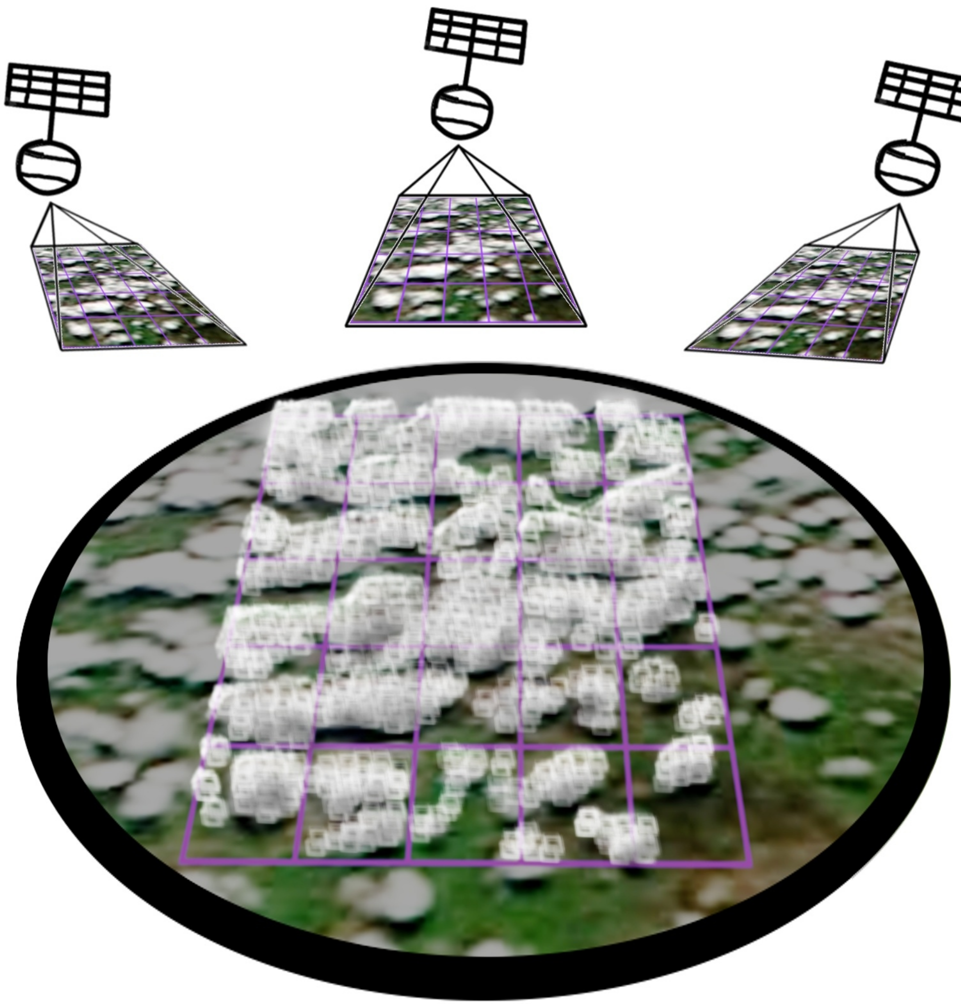
Three-dimensional cloud



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  X

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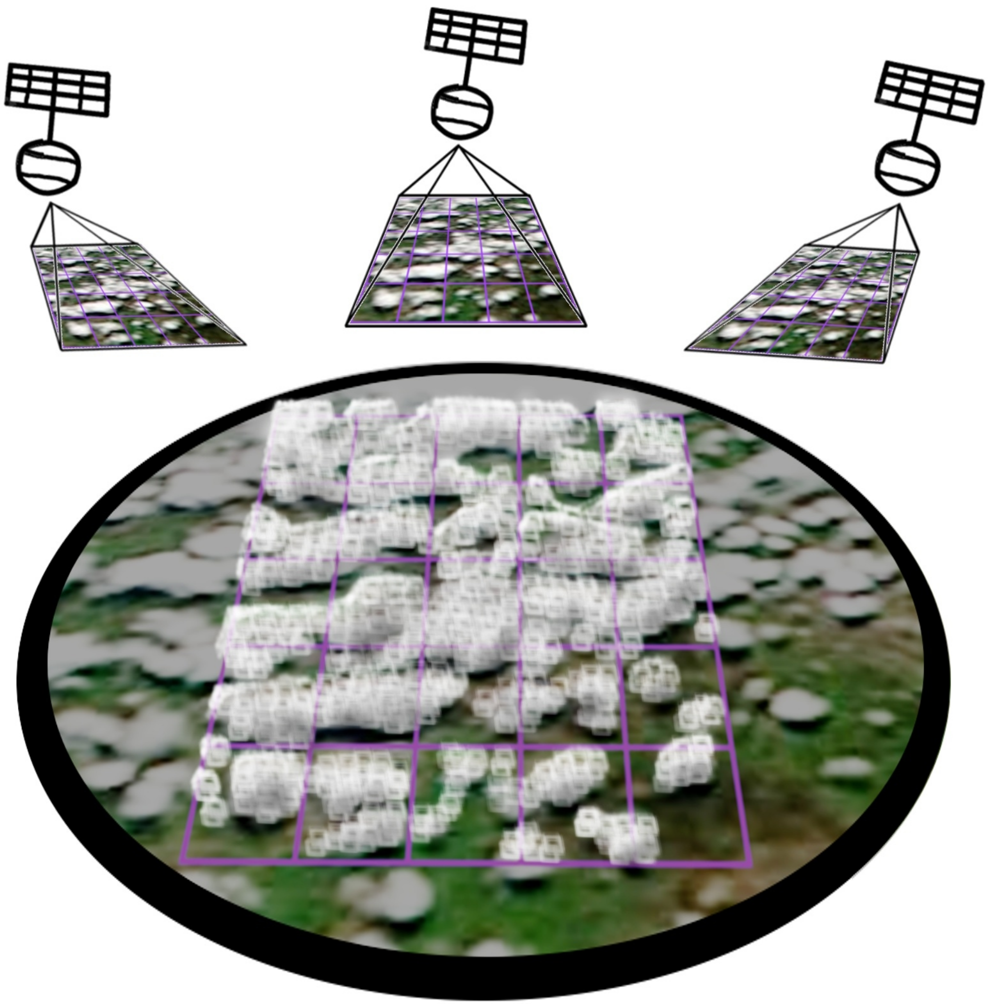
This gives a large scale inverse problem:
Adjust 10,000 unknowns to fit 1,000,000 data.

Inverse problem:
find the cloud which fits data "best"



Minimize the misfit

- Non-linear least squares problem
- Solve by iterative methods

Requires the evaluation of the

$$\Phi\left(\boldsymbol{a}\right) = \frac{1}{2}\left(\hat{\boldsymbol{y}} - \boldsymbol{y}(\boldsymbol{a})\right)^T \cdot \boldsymbol{S}_{\boldsymbol{\epsilon}}^{-1} \cdot \left(\hat{\boldsymbol{y}} - \boldsymbol{y}(\boldsymbol{a})\right)$$

And the derivative of the misfit (steepest descent)

$$-\frac{\partial\Phi(\boldsymbol{a})}{\partial a^n} = \left(\hat{\boldsymbol{y}} - \boldsymbol{y}(\boldsymbol{a})\right)^T \cdot \left(\boldsymbol{S}_{\boldsymbol{\epsilon}}^{-1}\right) \cdot \frac{\partial \boldsymbol{y}(\boldsymbol{a})}{\partial a^n}$$

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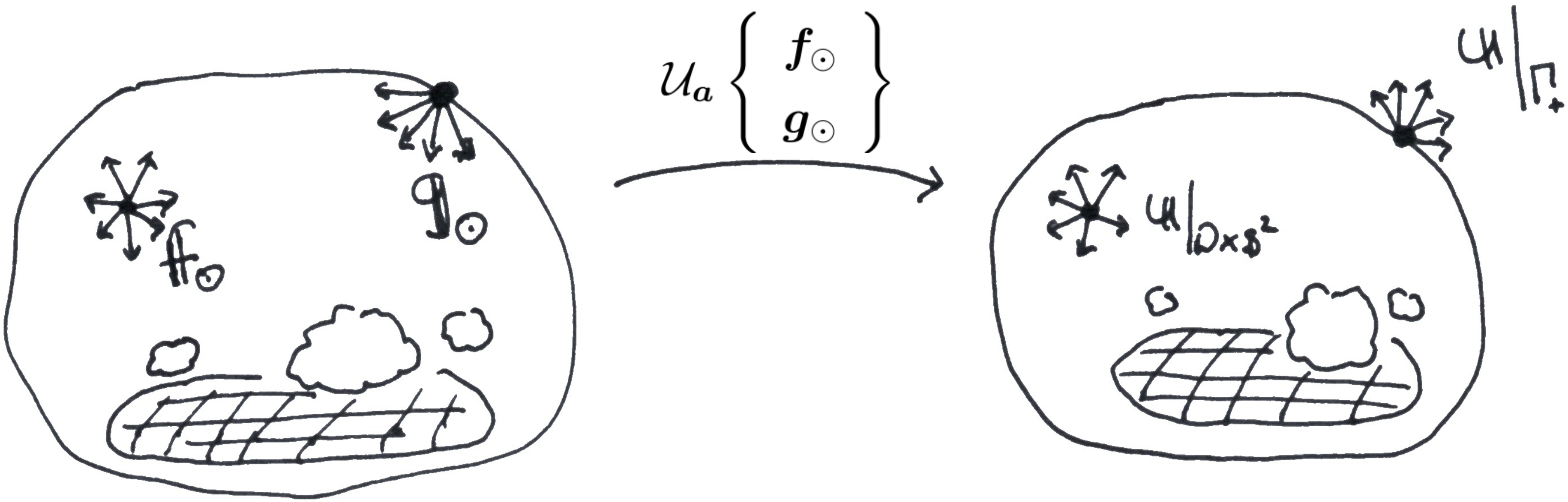
Adjoint method:
to evaluate y(a) we need a solver.

For a fixed atmosphere and surface, the solver transforms volume-source and incoming-source functions into the internal and outgoing Stokes vectors.



Boundary value problem for 3D Radiative Transfer

$$\begin{aligned} \boldsymbol{v}\cdot\nabla\boldsymbol{u} + \sigma\boldsymbol{u} - \mathcal{Z}[\boldsymbol{u}] &= \boldsymbol{f}_\odot \quad \text{on} \quad D\times\mathbb{S}^2, \\ \boldsymbol{u}|_{\Gamma_-} - \mathcal{R}\big[\boldsymbol{u}|_{\Gamma_+}\big] &= \boldsymbol{g}_\odot \quad \text{on} \quad \Gamma_-. \end{aligned}$$

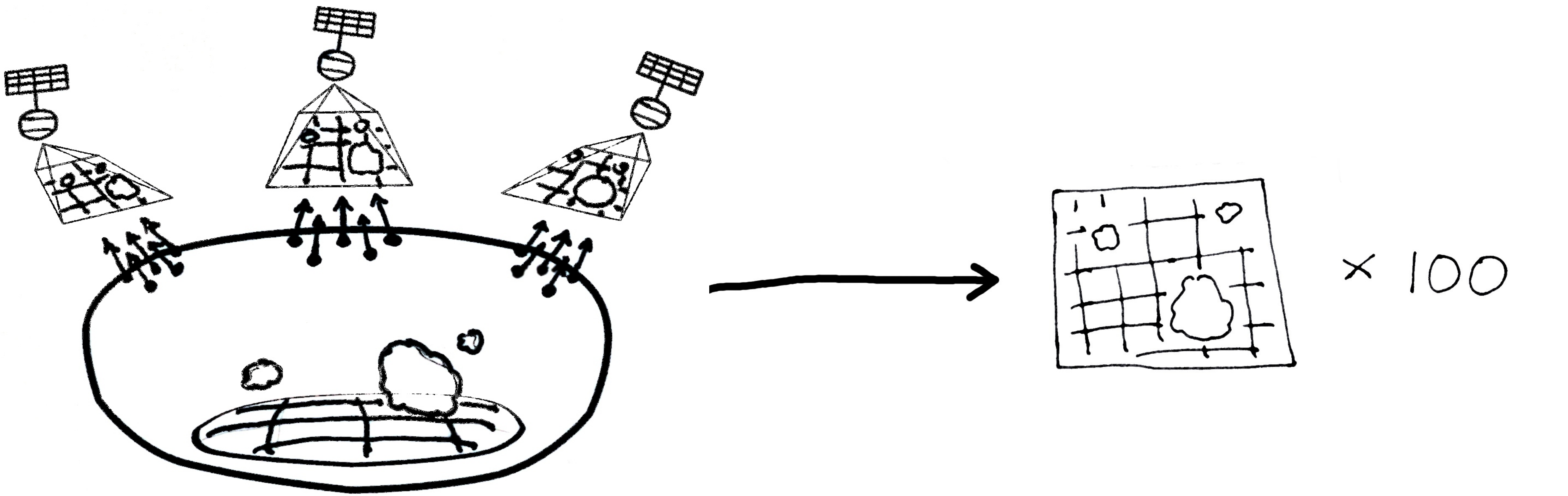
Solution operator (i.e. solver)

$$\left\{ \begin{array}{c} \boldsymbol{u}|_{D\times\mathbb{S}^2} \\ \boldsymbol{u}|_{\Gamma_+} \end{array} \right\} = \mathcal{U}_a \left\{ \begin{array}{c} \boldsymbol{f}_\odot \\ \boldsymbol{g}_\odot \end{array} \right\}$$

Adjoint method:

y(a) is a integral over the solution

Integrate the Stokes vector solution over the polarimetric response of each pixel.

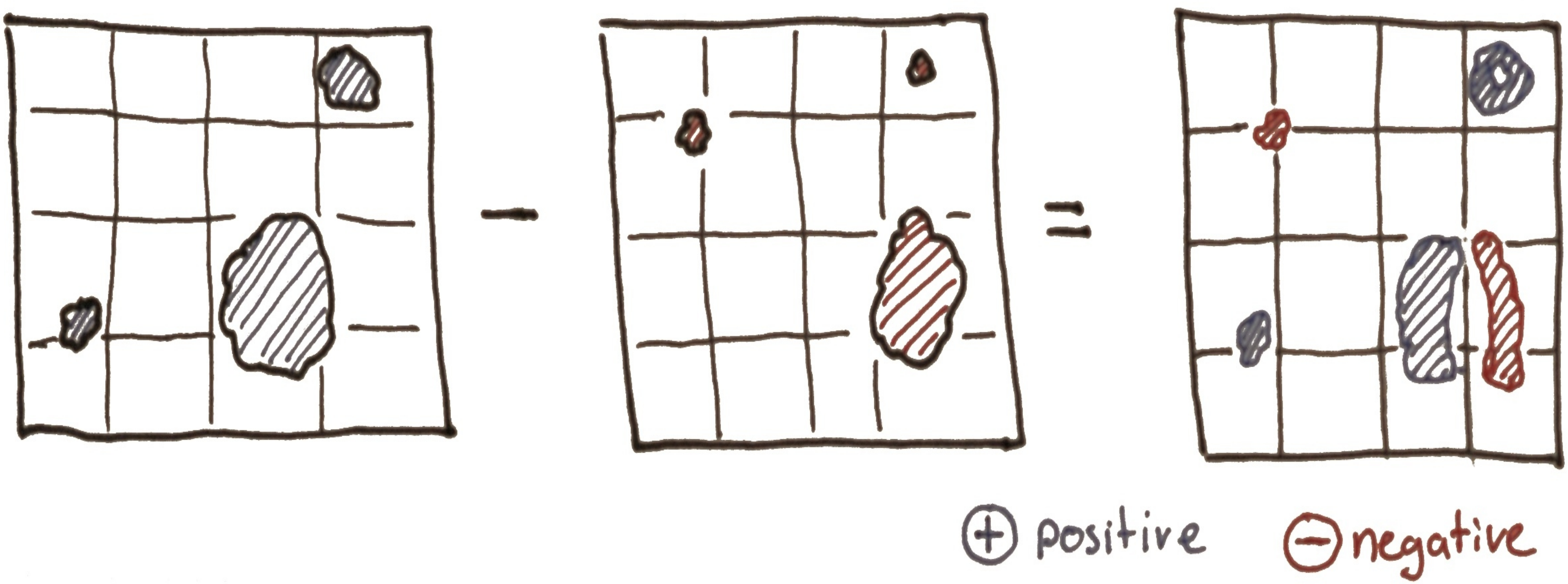


$$y^m(\boldsymbol{a}) = \left\langle \left\{ \begin{array}{c} \boldsymbol{p}_\odot^m \\ \boldsymbol{q}_\odot^m \end{array} \right\}, \mathcal{U}_{\boldsymbol{a}} \left\{ \begin{array}{c} \boldsymbol{f}_\odot \\ \boldsymbol{g}_\odot \end{array} \right\} \right\rangle_{D\times\mathbb{S}^2\oplus\Gamma_+}$$

Adjoint method:

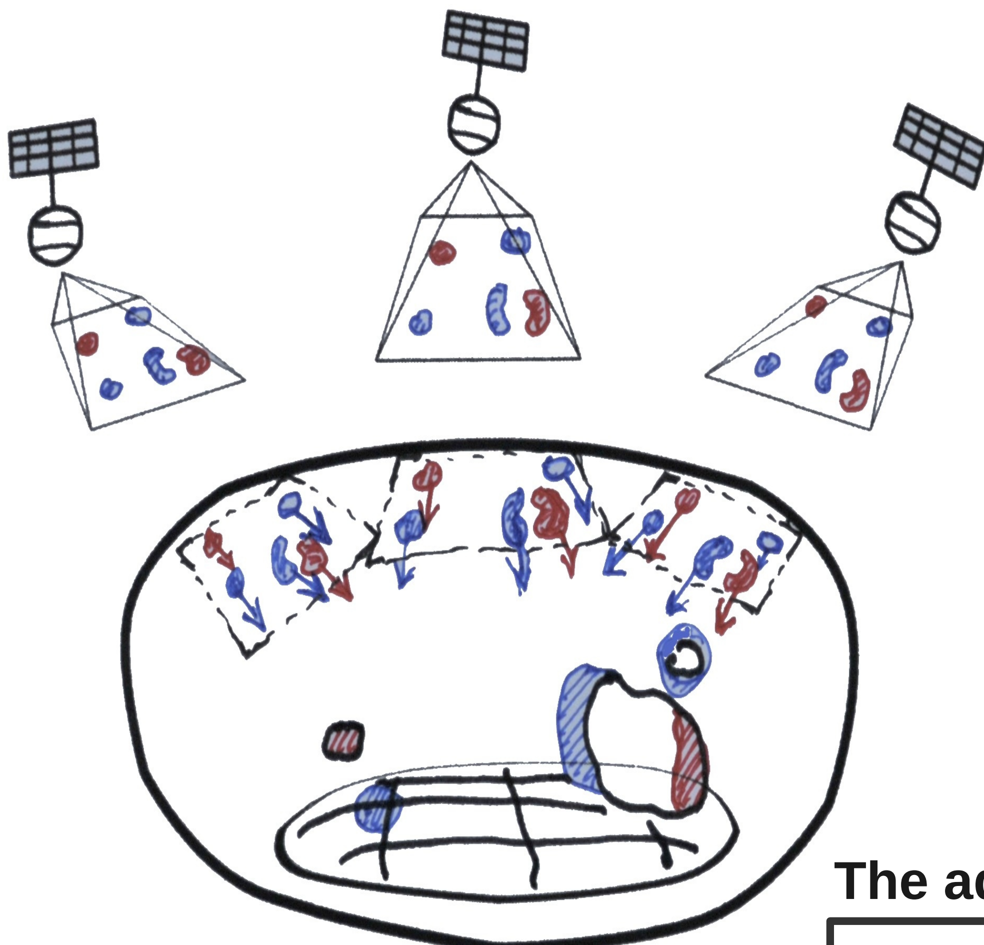
compute the measurement residual

y_{data} $\qquad$ $y(a)$



Adjoint method:

solve the adjoint 3D VRTE



The measurement residual is on the wrong domain

- 2D images in space

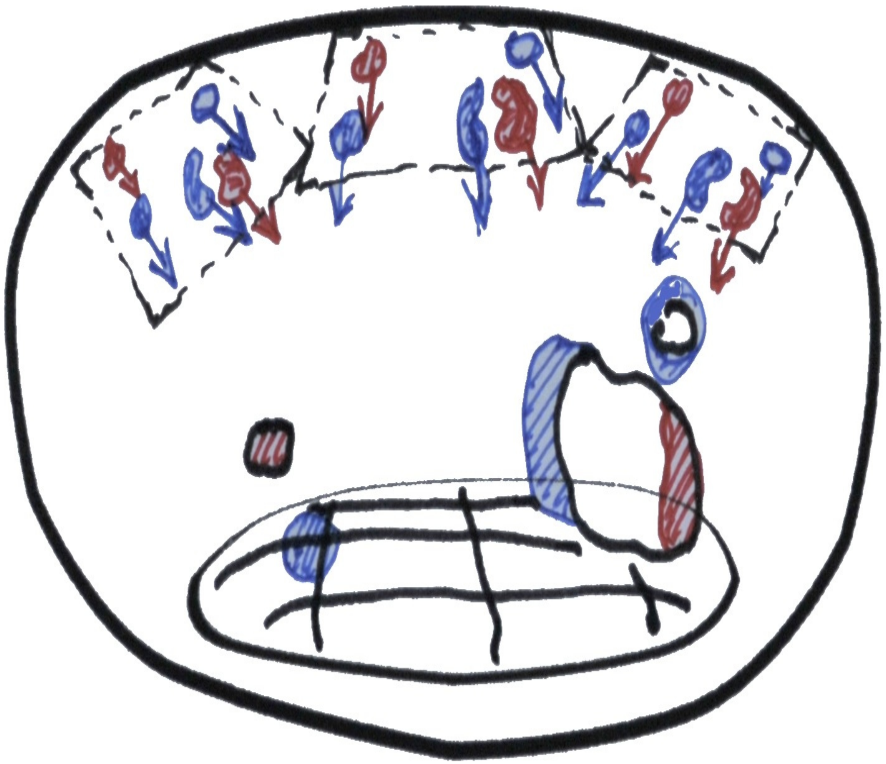
The adjoint solution is on the right domain

- 3D atmosphere and surface

The adjoint solver calls the forward solver

$$\boxed{\mathcal{U}_{\boldsymbol{a}}^{*}\left\{\begin{array}{c}\boldsymbol{p}_{\odot}\\ \boldsymbol{q}_{\odot}\end{array}\right\}=\alpha\boldsymbol{Q}\mathcal{U}_{\boldsymbol{a}}\left\{\begin{array}{c}\alpha\boldsymbol{Q}\boldsymbol{p}_{\odot}\\ \alpha\boldsymbol{Q}\boldsymbol{q}_{\odot}\end{array}\right\}}$$

Adjoint method:
compute the steepest descent of misfit



The adjoint Stokes-vector solution is on the correct 3D domain.

Compute the steepest descent of the misfit function.

- This is the right-hand-side of Newton's equations for the parameter adjustment.

$$-\frac{\partial \Phi}{\partial a^n} = \left\langle \mathcal{U}_{\boldsymbol{a}}^{*} \left\{ \begin{array}{c} \boldsymbol{\Delta p}_{\odot} \\ \boldsymbol{\Delta q}_{\odot} \end{array} \right\}, \left\{ \begin{array}{c} \boldsymbol{\Delta f}_{\odot}^{n} \\ \boldsymbol{\Delta g}_{\odot}^{n} \end{array} \right\} \right\rangle_{D\times\mathbb{S}^2 \oplus \Gamma_-}$$

Adjoint method:

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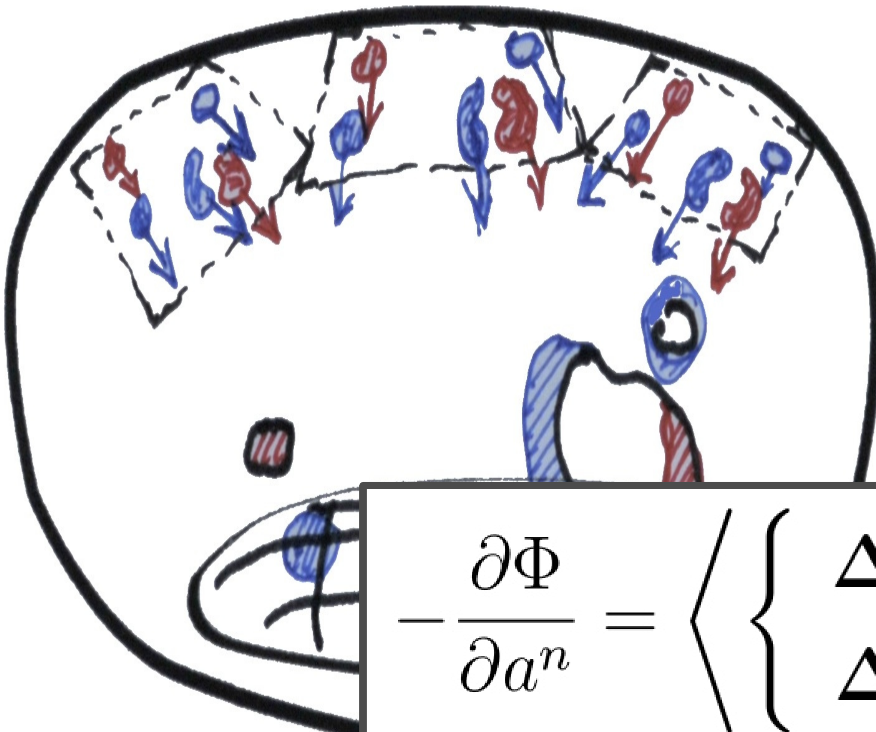

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$$-\frac{\partial \Phi}{\partial a^n} = \left\langle \mathcal{U}^*_{\boldsymbol{a}} \left\{ \begin{array}{c} \boldsymbol{\Delta p}_\odot \\ \boldsymbol{\Delta q}_\odot \end{array} \right\}, \left\{ \begin{array}{c} \boldsymbol{\Delta f}^n_\odot \\ \boldsymbol{\Delta g}^n_\odot \end{array} \right\} \right\rangle_{D\times\mathbb{S}^2\oplus\Gamma_-}$$

How do we tell the computer?

computers know linear algebra.

Use the derivative:

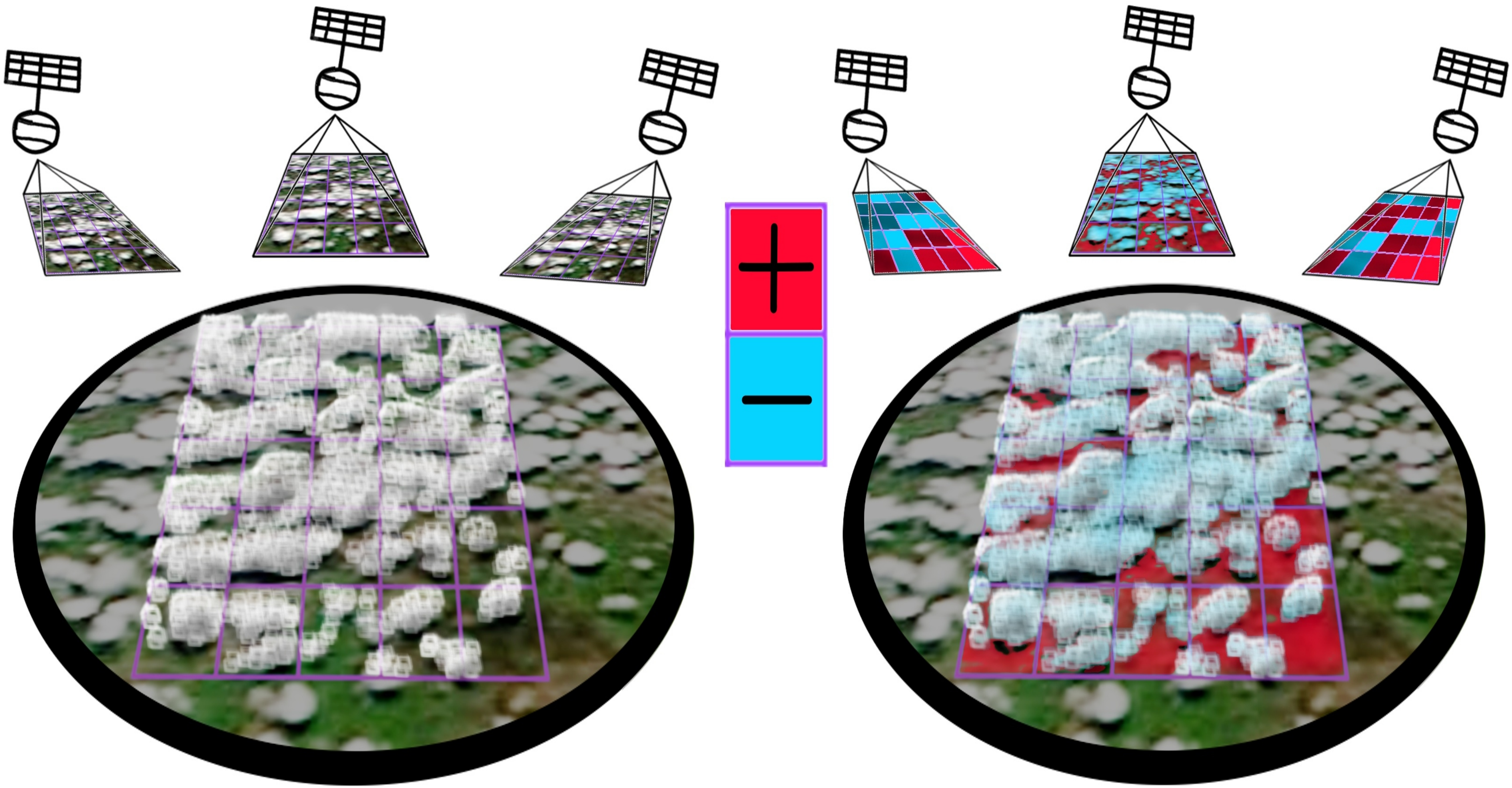
grad(Φ),

To setup the linear system:

Ax=b.

Adjoint method:

scalable adjustments to 3D properties



Adjoint method:
scalable adjustments to 3D properties

Iterative minimization of the misfit function with only two calls to the 3D VRTE (per wavelength):

- Solve the 3D VRTE once to compute the residual
- Solve the adjoint 3D VRTE once calculate the derivative
- Solve a system of linear equations for the parameter adjustment

Procedure scales to very large problems with . . .

- Many measurement constraints
- Many unknown cloud, aerosol and surface properties

Adjoint method makes 3D retrievals with the 3D VRTE worth discussing

- Future project 1: Test derivative calculations and performance
- Future project 2: Synthetic retrievals and inverse problem analysis

Adjoint methods for 3D
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Thank you!!!

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Adjoint method:

The adjoint source from residuals

Recall the expression for each measurement:

$$y^m(\boldsymbol{a}) = \langle \boldsymbol{p}^m_\odot, \boldsymbol{u} \rangle_{D\times\mathbb{S}^2} + \langle \boldsymbol{q}^m_\odot, \boldsymbol{u} \rangle_{\Gamma_+}$$

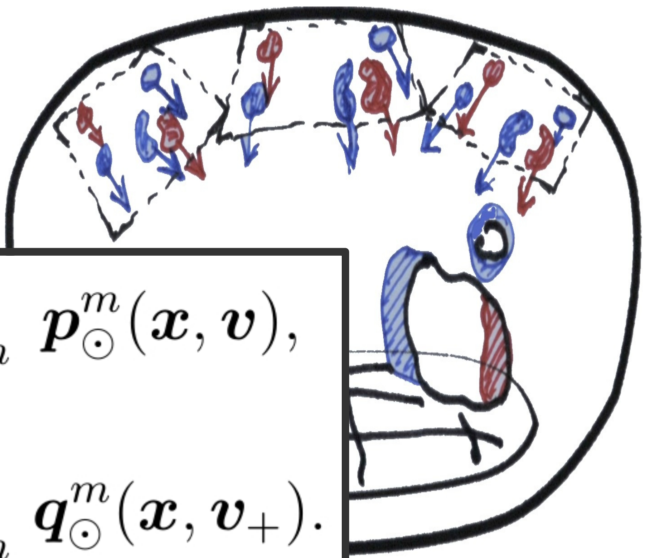
Avoid computing the Jacobian (sum over measurements first)

$$\begin{aligned} -\frac{\partial \Phi(\boldsymbol{a})}{\partial a^n} &= (\hat{\boldsymbol{y}} - \boldsymbol{y}(\boldsymbol{a}))^T \cdot (\boldsymbol{S}_\epsilon^{-1}) \cdot \frac{\partial \boldsymbol{y}(\boldsymbol{a})}{\partial a^n} \,. \\ &= \left\langle \boldsymbol{\Delta p}_\odot, \frac{\partial \boldsymbol{u}}{\partial a^n} \right\rangle_{D\times\mathbb{S}^2} + \left\langle \boldsymbol{\Delta q}_\odot, \frac{\partial \boldsymbol{u}}{\partial a^n} \right\rangle_{\Gamma_+} \end{aligned}$$

The adjoint source functions

$$\boldsymbol{\Delta p}_\odot(\boldsymbol{x}, \boldsymbol{v};\, \boldsymbol{a}) = \sum_{m'\,m} \left(\hat{y}^{m'} - y^{m'}(\boldsymbol{a})\right) \, \left(\boldsymbol{S}_\epsilon^{-1}\right)_{m'm} \, \boldsymbol{p}^m_\odot(\boldsymbol{x}, \boldsymbol{v}),$$

$$\boldsymbol{\Delta q}_\odot(\boldsymbol{x}, \boldsymbol{v}_+;\, \boldsymbol{a}) = \sum_{m'\,m} \left(\hat{y}^{m'} - y^{m'}(\boldsymbol{a})\right) \, \left(\boldsymbol{S}_\epsilon^{-1}\right)_{m'm} \, \boldsymbol{q}^m_\odot(\boldsymbol{x}, \boldsymbol{v}_+).$$



Adjoint method:
sources for parameter derivatives

Differentiate the VRTE:

$$\boxed{\frac{\partial}{\partial a^n}} \Rightarrow \boxed{\begin{aligned} \boldsymbol{v}\cdot\nabla\boldsymbol{u}+\sigma\boldsymbol{u}-\mathcal{Z}[\boldsymbol{u}] &= \boldsymbol{f}_{\odot} \\ \boldsymbol{u}|_{\Gamma_-}-\mathcal{R}\left[\boldsymbol{u}|_{\Gamma_+}\right] &= \boldsymbol{g}_{\odot} \end{aligned}}$$

3D VRTE with same left-hand-side:

$$\begin{aligned} \boldsymbol{v}\cdot\nabla\frac{\partial\boldsymbol{u}}{\partial a^n}+\sigma\frac{\partial\boldsymbol{u}}{\partial a^n}-\mathcal{Z}\left[\frac{\partial\boldsymbol{u}}{\partial a^n}\right] &= \boldsymbol{\Delta f}^n_{\odot}, \\ \left.\frac{\partial\boldsymbol{u}}{\partial a^n}\right|_{\Gamma_-}-\mathcal{R}\left[\left.\frac{\partial\boldsymbol{u}}{\partial a^n}\right|_{\Gamma_+}\right] &= \boldsymbol{\Delta g}^n_{\odot}, \end{aligned}$$

The derivative solves the 3D VRTE with the following right-hand-side source:

$$\begin{aligned} \boldsymbol{\Delta f}^n_{\odot}(\boldsymbol{x},\boldsymbol{v};\,\boldsymbol{a}) &= -\frac{\partial\sigma}{\partial a^n}(\boldsymbol{x};\boldsymbol{a})\;\boldsymbol{u}(\boldsymbol{x},\boldsymbol{v};\,\boldsymbol{a})+\frac{1}{4\pi}\int_{\mathbb{S}^2}\mathrm{d}S_{\boldsymbol{v}'}\;\frac{\partial\boldsymbol{Z}}{\partial a^n}(\boldsymbol{x},\boldsymbol{v},\boldsymbol{v}';\boldsymbol{a})\cdot\boldsymbol{u}(\boldsymbol{x},\boldsymbol{v}';\,\boldsymbol{a}) \\ \boldsymbol{\Delta g}^n_{\odot}(\boldsymbol{x},\boldsymbol{v}_-;\,\boldsymbol{a}) &= \frac{1}{2\pi}\int_{\boldsymbol{v}_+\cdot\nabla h(\boldsymbol{x})>0}\mathrm{d}S_{\boldsymbol{v}_+}\;\left|\boldsymbol{v}_+\cdot\nabla h(\boldsymbol{x})\right|\;\frac{\partial\boldsymbol{R}}{\partial a^n}(\boldsymbol{x},\boldsymbol{v}_-,\boldsymbol{v}_+;\boldsymbol{a})\cdot\boldsymbol{u}(\boldsymbol{x},\boldsymbol{v}_+;\,\boldsymbol{a}). \end{aligned}$$

Adjoint method:
sources for parameter derivatives

$$\begin{Bmatrix} \dfrac{\partial \boldsymbol{u}}{\partial a^n}\Big|_{D\times\mathbb{S}^2} \\ \dfrac{\partial \boldsymbol{u}}{\partial a^n}\Big|_{\Gamma_+} \end{Bmatrix} = \mathcal{U}_{\boldsymbol{a}} \begin{Bmatrix} \boldsymbol{\Delta f}^n_{\odot} \\ \boldsymbol{\Delta g}^n_{\odot} \end{Bmatrix}$$

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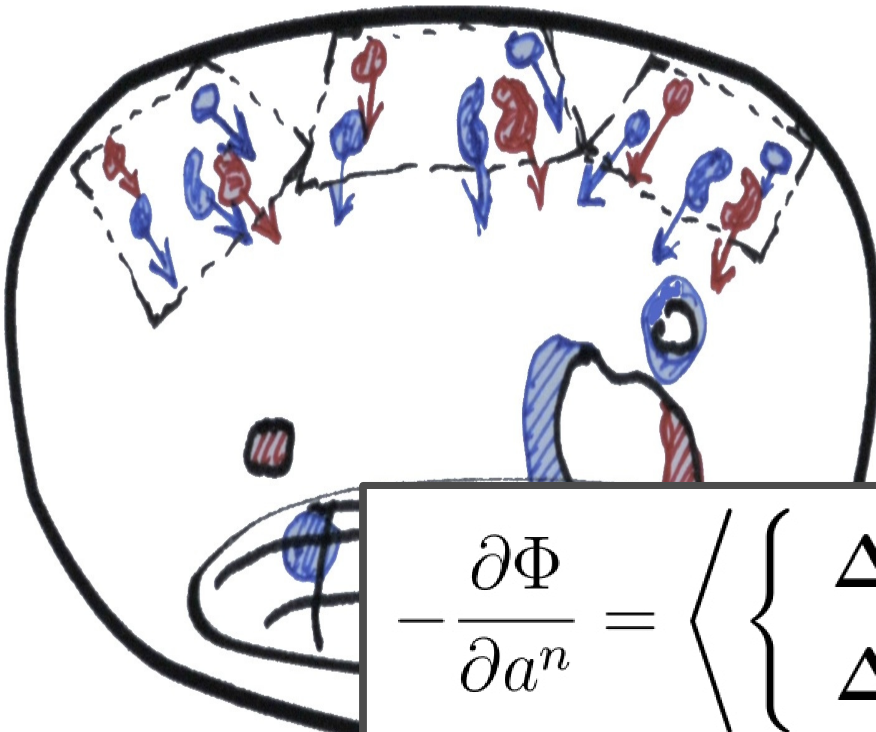
$$\boldsymbol{\Delta g}^n_{\odot}(\boldsymbol{x},\boldsymbol{v}_-;\,\boldsymbol{a}) = \frac{1}{2\pi}\int_{\boldsymbol{v}_+\cdot\nabla h(\boldsymbol{x})>0}\mathrm{d}S_{\boldsymbol{v}_+}\;\left|\boldsymbol{v}_+\cdot\nabla h(\boldsymbol{x})\right|\frac{\partial \boldsymbol{R}}{\partial a^n}(\boldsymbol{x},\boldsymbol{v}_-,\boldsymbol{v}_+;\boldsymbol{a})\cdot\boldsymbol{u}(\boldsymbol{x},\boldsymbol{v}_+;\,\boldsymbol{a}).$$

Adjoint method:
compute the steepest descent of misfit



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How do we tell the computer?

computers know linear algebra.

Adjust parameters with a step, b, which solves approximate Newton's equations:

$$\left(\nabla\nabla\Phi(\boldsymbol{a}) + \nabla\nabla\Phi_{\mathrm{prior}}(\boldsymbol{a})\right)\cdot\boldsymbol{b} = -\left(\nabla\Phi(\boldsymbol{a}) + \nabla\Phi_{\mathrm{prior}}(\boldsymbol{a})\right)$$

Approximate the second derivative with the gradient (Broyden-Fletcher-Goldfarb-Shanno):

$$\nabla\nabla\Phi(\boldsymbol{a}_k) \approx \boldsymbol{H}_k\left(\boldsymbol{a}_0, \cdots, \boldsymbol{a}_k, \nabla\Phi(\boldsymbol{a}_0), \cdots, \nabla\Phi(\boldsymbol{a}_k)\right)$$